3-Hexenoic acid, methyl ester

Other names: Methyl 3-hexenoate
methyl hex-3-enoate
Inchi: InChI=1S/C7H12O2/c1-3-4-5-6-7(8)9-2/h4-5H,3,6H2,1-2H3
InchiKey: XEAIHUDTEINXFG-UHFFFAOYSA-N
Formula: C7H12O2
SMILES: CCC=CCC(=O)OC
Mol. weight [g/mol]: 128.17
CAS: 2396-78-3

Physical Properties

Property code	Value	Unit	Source
gf	-145.64	kJ/mol	Joback Method
hf	-315.39	kJ/mol	Joback Method
hfus	16.88	kJ/mol	Joback Method
hvap	40.29	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.516		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3114.04	kPa	Joback Method
rinpol	933.00		NIST Webbook
rinpol	936.00		NIST Webbook
ripol	1234.00		NIST Webbook
tb	440.01	K	Joback Method
tc	625.03	K	Joback Method
tf	235.73	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.68	J/mol×K	440.01	Joback Method
cpg	272.15	J/mol×K	594.20	Joback Method
cpg	263.10	J/mol×K	563.36	Joback Method
cpg	253.64	J/mol×K	532.52	Joback Method

cpg	243.76	J/mol×K	501.68	Joback Method
cpg	233.44	J/mol×K	470.85	Joback Method
cpg	280.80	J/mol×K	625.03	Joback Method
dvisc	0.0002208	Pa×s	440.01	Joback Method
dvisc	0.0002837	Pa×s	405.96	Joback Method
dvisc	0.0003815	Pa×s	371.92	Joback Method
dvisc	0.0005447	Pa×s	337.87	Joback Method
dvisc	0.0008422	Pa×s	303.82	Joback Method
dvisc	0.0014537	Pa×s	269.78	Joback Method
dvisc	0.0029377	Pa×s	235.73	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.89075e+01
Coeff. B	-5.07474e+03
Coeff. C	-6.56080e+01
Temperature range (K), min.	338.15
Temperature range (K), max.	438.86

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2396783&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume